SURE Projects 2024

Email *

lunghia@tcd.ie

Project Title *

Spin decoherence in molecular qubits

Supervisor(s) *

Alessandro Lunghi

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

In recent years, quantum science has evolved from a fundamental theory used to explain physical phenomena, to an active player in modern technologies. The spin of electrons behaves as a prototypical 2-level quantum system and therefore represents the ideal quantum bit (qubit), i.e. the logical unit of a quantum machine. In this project the student will use state-of-the-art quantum mechanical calculations to describe the time evolution of the quantum states associated with the spin of a magnetic molecule, namely a molecular qubit.

Students tasks *

The project is computational in nature. The student will use the Python library PyCCE to efficiently simulate the evolution of the spin state of a series of magnetic molecules. The intern will also develop Python script to analyze and interpret the results obtained with PyCCE. The student will regularly meet with the supervisor and will take part to the supervisor’s group activities, such as group meetings and seminars.

Essential prerequisites

Basic knowledge of python

SURE Projects 2024

Email *

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Project Title *

Simulting hte quantum tunneling of molecular magnetizationn

Supervisor(s) *

Alessandro Lunghi

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

The magnetization of single molecules exhibit quantum mechanical features, making it possible to probe quantum mechanical effects for nanoscale and larger objects. In particular the magnetization of single molecules have been show tunneling effects, where it can reverse its direction without exploring intermediate orientation. On the one hand, the study of this effect opens a window on fundamental questions about quantum mechanics. On the other hand, it paves the way to the control of molecular magnets for high density information storage and quantum bits. Until now, the theoretical desription of magnetization tunneling have been confined to phenomenological models and no first-principles description of this process is available.

Students tasks *

The student will use existing FORTRAN libraries developed by the supervisor's group in order to simulate the quantum dynamics of molecular spins entangled among them through dipolar interactions and exhibiting tunneling phenomena. The novel software will implement correlated cluster expansion methods in order to make the problem computationally feasable. The student will familiarize themselves with quantum dynamics models and will learn to write scientific software and execute it on large-scale computational facilities.

Essential prerequisites

Basic knowledge of at least one programming language; Understanding of the fundamental principles of quantum mechanics

SURE Projects 2024

Email *

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Project Title *

Geometry matters at the nanoscale

Supervisor(s) *

Majid Fazeli, Graham Cross

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

The mapping of inelastic mechanical properties like hardness at sub 100 nm scales is a major hurdle yet to be overcome in nanoscience, and is vital for emerging nanotechnologies. In this project, you will used advanced finite element modeling to help interpret the results of new diamond atomic force microscopy (AFM) probes to perform high speed hardness measurements at the 1-100 nm scale. Your simiulations will be matched to multi-dimensional nanoindentation results from our lab to help bring a new regime of property mapping to scanning probe instrumentation.

Students tasks *

1. Learn how to run explicity finite element simulations using the Abaqus package
2. Build 2D then 3D models of diamond micro-cantilevers with Berkovich shape indenter tips
3. Conduct indentation exerperiment simulations of standard sample materials like fused silica, aluminium, tungsten and silicon to understand the nature of deformation, forces and how to compensate for parasitic loadings in the challenging AFM configuration

Essential prerequisites

Affinity for computer programming and simulations, interest in solving real-world problems

SURE Projects 2024

Email *

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Project Title *

An energy approch to generate Truchet tilings

Supervisor(s) *

Stefan Hutzler

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Truchet tiling refers to the tiling of a plane with squares that are composed of two triangles of different colours. The tiles can be placed in four different orientations. The tilings that can be achieved with such tiles may be anything between ordered arrangements of various complexity or completely random patterns.

This computational project will produce such tilings (for example using Mathematica) using an “energy”-based algorithm. Each arrangement will be associated with a numerical energy value, computed from some user-defined energy functional. The functional could for example be the sum of all black triangles that meet at every vertex (ie the meeting point of four tiles), or it could take into account the character also of neighbouring vertices. For a given energy functional, a minimisation algorithm, for example simulated annealing combined with tile rotation, will be used to find a tiling of minimal energy.

Reference
Smith, C.S. and Boucher, P., 1987. The tiling patterns of Sebastien Truchet and the topology of structural hierarchy. Leonardo, 20(4), pp.373-385.
https://en.wikipedia.org/wiki/File:Truchet_ordered_tiling.svg

Students tasks *

Writing code for the generation of such tilings. Mathematica software is available for this which would serve as a good starting point. Exploration of different energy functionals and minimisation techniques. Assessment of the produced patterns.

Essential prerequisites

A love of performing computer simulations.

SURE Projects 2024

Email *

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Project Title *

Combining machine-learning and clever representations to solve the Schroedinger equation

Supervisor(s) *

Stefano Sanvito

Type of project *

- (●) Theoretical
- ( ) Computational
- ( ) Experimental

Project description *

In this project we will explore different ways to expand the wave-function and the necessary operators (e.g. the Hamiltonian) in order to construct an efficient numerical solution of the Schoedinger equation. In particular, we will consider delocalised basis sets with appropriate boundary conditions (e.g. the Legendre polynomials). One of the goals is to identify the best numerical platform for integrating standard electronic structure methods with machine learning, in particular for the construction of approximated form of the kinetic energy. This is one of the most sought-after quantity in modern electronic structure theory.

Students tasks *

The project is really end-to-end (the student will be in control of every aspect). The student will write a complete Python code to solve the Schroedinger equation. For simplicity we will consider the case of 1D particle in a box, with random Gaussian potential. The problem will be expanded over different basis set and solved numerically. We will compare the efficacy of different wave-funciton representation.

Essential prerequisites

Quantum mechanics; Python coding (not necessarily advanced).

SURE Projects 2024

Email *

sanvitos@tcd.ie

Project Title *

Optical character recognition for machine-learning data extraction

Supervisor(s) *

Stefano Sanvito

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Advances in the development of large language models (e.g. ChatGPT) has taken many technology areas by storm. Physics and materials science are not excluded from this revolution. For instance, large language models can be used to extract precise information from scientific literature and this can be used to construct machine-learning models to predict properties of materials. In a nutshell one can use large language models to "read" papers at a speed that humans cannot even think about (250,000 papers per week). This project will atempt at using optical character recognition methods to construct machine-learning models able to understand tables from a scientific paper. This is a tricky task, since the table structure and its caption, in addition to its content, define the information to extract.

Students tasks *

Use optical character recognition libraries as platform for machine-learning models to extract data from tables. The student will consider different available libraries and evaluate their accuracy and precision in extracting information from table. S/he will construct machine-learning models to optimize the task and methods to evaluate performace and errors.

Essential prerequisites

Ability to read a scientific paper; Coding in Python.

SURE Projects 2024

Email *

hozhang@tcd.ie

Project Title *

Controllable growth of two-dimensional MoS2 films with desirable grain structures

Supervisor(s) *

Hongzhou Zhang

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

Two-dimensional (2D) transition-metal-dichalcogenides (TMDs) have attracted considerable interest in the research community for their potential applications in electronics and optoelectronics. High quality wafer-scale monolayer or few-layer TMD films have been extensively demonstrated using chemical vapour deposition (CVD). CVD films are usually polycrystalline with grains of random sizes and orientations, while the grain structure dominates the properties of the film. For example, grain boundaries are responsible for the resistive switching in 2D MoS2 memristors when an electric field is applied. However, since the functionality and performance of the device rely on randomly oriented grains, such a device is not scalable and hence has limited real-world applications regardless of its unique and promising properties. Therefore, it is imperative to realise controllable growth of two-dimensional MoS2 films with desirable grain structures.

The Zhang group has discovered a new approach to mediating the nucleation of MoS2 growth via substrate patterning. In this project, we will investigate the effects of substrate patterning on the grain structure of the 2D MoS2 films. We will use optical lithography to pattern the substrate and conduct chemical vapour deposition. A range of advanced characterisation methods (e.g. scanning electron microscopy, atomic force microscopy, Raman spectroscopy and photoluminescence) will be employed to investigate the morphologies of the films.

Students tasks *

CVD growth; Optical characterisation

Essential prerequisites

Basic lab skills

SURE Projects 2024

Email *

hozhang@tcd.ie

Project Title *

p-type doping of two-dimensional MoS2 films

Supervisor(s) *

Hongzhou Zhang

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

The success of modern electronics relies on transistor scaling, but the reduction of the dimensions of silicon transistors has encountered insurmountable obstacles. Two-dimensional (2D) transition-metal-dichalcogenide (TMD) based transistors have recently become a promising candidate to further device scaling. Prototype 2D TMD-based transistors show superior performance (e.g. high mobility, large ON/Off ratio, reduced short channel effects, improved gate modulation and low power consumption). For device applications, it is of importance to modulate the type and concentration of the majority charge carriers in the channel. However, bipolar doping of 2D TMDs remains a challenge because their natural doping propensity leads to unipolar conduction.
The Zhang group have invented a polymer-assisted chemical vapour deposition (CVD) method for wafer-scale 2D TMD fabrication. In this project, we will develop the CVD method and explore p-type doping of few-layered MoS2. We will fabricate 2D MoS2 transistors and investigate the doping effects

Students tasks *

CVD growth; Raman/PL XRD characterisations

Essential prerequisites

Basic lab skills

SURE Projects 2024

Email *

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Project Title *

Exoplanet Weather: Cloudy with a Chance of Molten Iron

Supervisor(s) *

Johanna Vos

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Imaged exoplanets and free-floating extrasolar worlds provide a direct and unique view into exoplanet atmospheres. Advanced telescopes such as the James Webb Space Telescope provide data of unprecedented quality, but the interpretation of this data relies on a thorough understanding of complex weather phenomena. In this project, the student will fit state-of-the-art atmospheric models to newly observed data JWST for a variety of giant extrasolar worlds to reveal their atmospheres in detail, including the composition of clouds and presence of molecules such as water and methane.

Students tasks *

The student will learn to access and visualise data from the Mikulski Archive for Space Telescopes. By comparing with the literature the student will learn to identify the dominant molecules in the atmosphere by eye. Finally, the student will turn to atmospheric models to arrive at a comprehensive view of each extrasolar atmosphere.

Essential prerequisites

Experience with python

SURE Projects 2024

Email *

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Project Title *

Sculpting the Physical properties of complex media: a multi-scale approach to material design

Supervisor(s) *

Mauro Ferreira

Type of project *

- (●) Theoretical
- ( ) Computational
- ( ) Experimental

Project description *

Details can be found here: https://www.dropbox.com/scl/fi/c41brt9aoxhgbjqpztv0x/SURE-Project-2024-MF.pdf?rlkey=wcgb2j182oml0afaoozwzlrvm&dl=0

Students tasks *

Details can be found here: https://www.dropbox.com/scl/fi/c41brt9aoxhgbjqpztv0x/SURE-Project-2024-MF.pdf?rlkey=wcgb2j182oml0afaoozwzlrvm&dl=0

Essential prerequisites

SURE Projects 2024

Email *

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Project Title *

Atmospheres of alien worlds: exploring new tools for spectroscopy of exoplanets

Supervisor(s) *

Neale Gibson

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Exoplanets are simply planets that orbit stars other than our Sun, and thousands have been discovered over the last few decades. A key frontier for astronomers is to try and characterise these planets in detail through spectroscopy of their atmospheres, which allows us to measure atmospheric temperatures and compositions, which in turn allows us to figure out the main physical and chemical processes that shape these worlds. The long term goal is to apply these methods to potentially habitable worlds, and even to search for 'biomarkers' - signs of extraterrestrial life.

Students tasks *

This project will use data from the James Webb Space Telescope (JWST) or a large ground-based facility like ESO’s Very Large Telescope to extract a spectrum of an exoplanet, allowing us to probe the chemistry and physical properties of the atmosphere. This project will focus on data analysis and statistics. The student will spend most of their time writing python code to analyse light curves and/or time-series spectra to extract an exoplanet's spectrum. Depending on the interests of the student, there may also be opportunities to study atmospheric physics and apply modelling techniques to understand the atmosphere.

Essential prerequisites

Knowledge of computer programming is essential. Experience of python would be valuable.

SURE Projects 2024

Email *

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Project Title *

Constraining the explosion mechanisms of Type Ia supernovae

Supervisor(s) *

Prof. Kate Maguire

Type of project *

- ○ Theoretical
- ◉ Computational
- ○ Experimental

Project description *

Type Ia supernovae, the explosions of white dwarfs in binary systems, are used in cosmology to determine distances in the Universe because they behave like standardisable candles. However, we still do not understand how they explode and there are many competing theories. In this project, the student will use data from the world-leading Zwicky Transient Facility, combined with new spectral data from ESO's Very Large Telescope, to link their observed light curves to their underlying explosion models by measuring the total mass of the ejecta. The aim is then to compare the estimated total masses to the predictions of different explosion channels for Type Ia supernovae to determine the most likely explosion scenario and improve sample selection for next-generation cosmological measurements.

Reference: [1] Scalzo R et al., 2014, MNRAS, 445, 2535, https://ui.adsabs.harvard.edu/abs/2014MNRAS.445.2535S/abstract

Students tasks *

This project is computational in nature and will involve Python coding to analyse the telescope data, estimate bolometric luminosities, and compare to explosion models and the literature. Machine-learning based algorithms and advanced statistical techniques [e.g., 2] can be introduced when investigating the link with the explosion models if the student is interested. The TCD transients research group is diverse and we strive for an friendly and collaborative working environment, with weekly group meetings and research discussions.

Reference: [2] Wojtak R. et al., 2023, MNRAS, 525, 5187, https://ui.adsabs.harvard.edu/abs/2023MNRAS.525.5187W/abstract

Essential prerequisites

SURE Projects 2024

Email *

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Project Title *

The conductivity of disordered, metallic flake packings

Supervisor(s) *

Matthias Mobius

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

In order to understand the conductive properties of 2D nanoparticle (e.g. graphene) films used in printed electronics you will explore a macroscopic model system of conducting metallic, high aspect ratio flakes to measure the axial and transverse conductivity as a function of volume fraction. You will study how the aspect ratio of the particles will influence the electronic transport properties.

Students tasks *

Sample preparation, 4-point resistance measurements

Essential prerequisites

Knowledge of electrical resistance and conductivity

SURE Projects 2024

Email *

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Project Title *

Photoemission spectroscopy and electronic structure of on-surface synthesised nanostructures or bilayers

Supervisor(s) *

Cormac McGuinness

Type of project *

- ○ Theoretical
- ○ Computational
- ◉ Experimental

Project description *

The project involves the use of x-ray photoemission spectroscopy methods (XPS) to characterise a number of differing in-situ grown materials and a study of their electronic and stoichiometric structure vi core-level spectroscopy and other surface science methods. The materials under study include on-surface synthesised nanostructures arising from porphyrin precursor materials on gold growth surfaces or bimetallic overlayers of transition metals on ruthenium surfaces in order to study their low temperature oxidation and reduction behaviours. Data analysis, fitting and some aspects of electronic structure simulation will be employed as well as significant laboratory work.

Students tasks *

Tasks include: the use of organic and/or metal evaporators on ultra high vacuum (UHV) equipment; the preparation of atomically clean surfaces; the deposition of thin films; the measurement of the XPS spectra using both newer and older generation XPS spectrometers; surface dosing and annealing of samples, and all steps leading up to such measurements. Notably this will also include assembly, disassembly and maintenance of UHV equipment inclusive of the testing of high temperature manipulators and sample transfer systems and bakeout of UHV equipment to obtain ultra high vacuum. Data analysis and simulation of electronic structure are also intended to be a significant part of the project and tasks.

Essential prerequisites

A desire to get your hands 'clean' when working with ulta-high vacuum equipment.